

# National Institute on Drug Abuse

## College on problems of drug DEPENDENCE

2006 - Scottsdale, Arizona

Scottsdale Princess Hotel

Salon I

Monday June 19, 2006

8:00 pm – 9:30 pm

### Workshop on hts and pubchem: nuts and bolts

*Christine Colvis, Ph.D., Chair*

**David Weaver, Ph.D.      “How to Do High Throughput Screening”**

**Tudor Oprea, M.D., Ph.D.    “How to Access and Use PubChem”**

The first workshop speaker, Dr. David Weaver, is the Director of the Vanderbilt Institute of Chemical Biology's High-throughput Screening Center (HTS) and the Principal Investigator of the Vanderbilt Screening Center for GPCRs, Ion Channels and Transporters. The latter center is a member of the ten-member Molecular Libraries Screening Center Network, funded through the NIH Roadmap Initiative. This network of screening centers provides resources for investigators interested in discovering chemical tools to support their research.

Dr. Weaver's presentation will focus on the utility of HTS of chemical libraries to discover molecular tools to promote advancement of basic and translational research programs. Principles of HTS assay design, validation, execution and analysis will be discussed. The workshop will provide participants with a chance to: (1) learn about and discuss how HTS might be useful for their research programs and (2) available funding opportunities for developing HTS screens and accessing the NIH Roadmap HTS infrastructure.

The second workshop speaker, Dr. Tudor Oprea, is the Chief of the Division of Biocomputing at the University of New Mexico School of Medicine, and co-PI of the New Mexico Molecular Libraries Screening Center. This center is a member of the Molecular Libraries Screening Center Network, funded through the NIH Roadmap Initiative, aimed at providing novel chemical probes for life sciences.

Dr. Oprea's presentation will highlight the tools available in PubChem (<http://pubchem.ncbi.nlm.nih.gov/>) with a focus on the retrieval of high throughput screening actives from the Small Molecule Repository. Examples of queries using PubChem Compound, PubChem Substance, PubChem Bioassay and Structure Search will be discussed. The workshop will provide participants with a chance to learn about and discuss how publicly available cheminformatics tools might be useful for their research programs and how novel chemical probes can shape new directions for research.

**Pre-registration is required, There is no pre-registration fee to attend this event, however participants will be accommodated on a first come, first served basis.**

**To pre-register, please contact Holly Buchanan at**

**[hbuchana@nida.nih.gov](mailto:hbuchana@nida.nih.gov) by June 1, 2006.**